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THE ENERGY DISPERSION OF THE SINGLET CORRELATED IMPURITY BAND IN LAYERED CUPRATES

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The Green's function method is applied to the calculation of the low energy spectrum in layered cuprates using Hubbard projection operators. Hund's and Kondo-like exchange, copper-oxygen and oxygen-oxygen hopping are taken into account. An analytical expression for the impurity band has been obtained. This expression is analysed in connection with considerations of Zhang and Rice, Matsukawa and Fukuyama and others that serve as the basis of the so-called t-J model.

1. INTRODUCTION

The problem of low lying excitations and mid-gap states is one of the central objects of interest in High-T_c Superconductivity[1]. According to Zhang and Rice[2] these properties are connected with the formation of local singlet copper-oxygen holes when adding the latter one into the CuO_2 plane by doping. Matsumoto, Sasaki and Tachiki[3] give important arguments for a new narrow band, which arises inside the charge transfer gap due to many body effects. There are some photoemission data ([4,5] and references therein) that lend considerable support to the existence of the narrow band near the Fermi level. Unfortunately, as it was already pointed out by Rice[6], the perturbation theory fails in it's usual form for the p-d mixing model because the transfer integral is comparable with the energetical distance from the lower Hubbard band. This is one of the reasons why the energy dispersion of this "impurity" band is still unknown. Additionally it is still an open question how it is connected with the singlet excitation. Recently this problem was discussed by Hayn, Yushankhai and Lovtsov[7].

The low energy spectrum is very sensitive to the values of the transfer integrals in the CuO_2 plane and especially to the values of the exchange coupling between copper and oxygen holes (Kondo exchange) as stressed by Fukuyama and Matsukawa[8]. In this context the present paper is organized as follows. At first we will derive a more accurate expression for the exchange coupling between copper and oxygen holes including the intraatomic exchange at the copper site (Hund's exchange). Then we will construct the 4x4 secular equation for the spectra including the lower Hubbard bands of Cu(2), O(2), O(3) and the Zhang-Rice excitations. After that we'll apply a new perturbation variant with the perturbation parameter w^s/Δ_1 where w^s is the singlet band width of about 0.2 eV and Δ_1 is the charge transfer gap of about 2 eV. We check our approach by exact numerical diagonalizations of the 4x4 eigenvalue equation.

2. MODEL HAMILTONIAN

In this section we present the interactions considered in the Hubbard Hamiltonian using Hubbard projection operators $p_{j\sigma}$, $d_{i\sigma}$ in the hole picture. The vacuum state $|0>$ corresponds to Cu^+. $d^+_{i\sigma}$ and $p^+_{j\sigma}$ are the creation operators of plane Cu^{2+} holes $|d_{x^2-y^2}>$ and O^- holes $|p_\sigma>$, respectively. The subscripts i and j denote the position of atoms in the CuO_2 plane. The energy difference between $|p_{j\sigma}>$ and $|d_{i\sigma}>$ states is Δ_1. The Coulomb repulsions of holes at the copper and oxygen site amount $U_{dd} \sim 9$ eV and $U_{pp} \sim 6$ eV, respectively([8] and references therein). The transfer integrals as defined in Fig. 1 are given by $t_\sigma \sim 1.2$ eV, $t^{xy} \sim 0.6$ eV and $t^{xx} \sim 0.4$ eV[8]. To examine the low energy physics we start from the following Hamiltonian:

$$H = \epsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \epsilon_p \sum_{j\sigma} p^+_{j\sigma} p_{j\sigma} + \sum_{ij} t^{pd}_{ij} (d^+_{i\sigma} p_{j\sigma} + p^+_{j\sigma} d_{i\sigma}) + \sum_{jj'} t^{pp}_{jj'} p^+_{j\sigma} p_{j'\sigma} + (V_{pd} - K_{pd}) \sum_i \psi^+_i \psi_i. \quad (1)$$

The last term on the r.h.s. contains the Coulomb repulsion $V_{pd} \sim 1$ eV[8] and the exchange interaction K_{pd} of holes in the local Zhang-Rice singlet (ZRS),

$$\psi_i = \frac{1}{\sqrt{2}} (P_{i\uparrow} d_{i\downarrow} - P_{i\downarrow} d_{i\uparrow}). \quad (2)$$

The linear combination $P_{i\sigma}$ of the four p_σ oxygen hole states around a copper hole $|d_{x^2-y^2}>$ state is[2]

$$P_{i\sigma} = \frac{1}{2} (p^{(1)}_{i\sigma} - p^{(2)}_{i\sigma} - p^{(3)}_{i\sigma} + p^{(4)}_{i\sigma}). \quad (3)$$

Now we are going to determine the energy spectrum by means of the equations of motion for the Greens functions. This method allows the use of a nonorthogonal basis immediately. That is why we do not need to construct the orthogonal basis set of Wannier functions as has been done by Zhang and Rice[2]. The expression for K_{pd} is given by:

$$K_{pd} = t^2_\sigma \left[\frac{6}{U_{dd} - \Delta_1 - 2V_{pd}} + \frac{1}{U_{dd'} - \Delta_2 - 2V_{pd}} + \frac{1.5}{U_{pp} + \Delta_1} \right] \quad (4)$$

It is caused by the virtual exchange via the upper copper and oxygen Hubbard bands only. In contrast to Zhang and Rice [2], Matsukawa and Fukuyama[8] and other authors we prefer to exclude any terms, which are proportional to t^2_σ/Δ_1 at the present stage. These terms would appear in a Kondo-like exchange if we would have used usual perturbation theory, but the latter one fails